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Diamond Light Source Proceedings / Volume 1 / Issue MEDSI-6 / October 2011 / e23
DOI: 10.1017/S2044820110000377, Published online: 26 October 2010

Link to this article: http://journals.cambridge.org/abstract_S2044820110000377

How to cite this article:

A. Gambitta (2011). A double crystal monochromator with self-compensation mechanism for ELETTRA XRD2 beamline. Diamond Light Source Proceedings, 1, e23 doi:10.1017/S2044820110000377

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Poster paper

A double crystal monochromator with self-compensation mechanism for ELETTRA XRD2 beamline

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(Received 17 June 2010; revised 31 August 2010; accepted 22 September 2010)

A prototype of a new double crystal monochromator (DCM) has been designed and developed for the second crystallography beamline (XRD2) at ELETTRA. The new device has to cover the 8–35 keV X-ray range. Since the corresponding diffraction angles are quite small, the choice has been to design a DCM with a fixed distance between the two crystals. As a consequence, the output beam has a small vertical displacement during the scan. This movement is compensated by means of an upstream mask, vertically moving and cutting the input beam at different heights. The movement of the mask is driven by a mechanism linked to the primary rotation of crystals (self-compensation), without any additional motor and following the displacement law required for compensation. The principle, the mechanism and the general mechanical concept of the device will be described in this paper.

1. Introduction

The monochromator is one of the key elements of the new hard X-ray beamline (XRD2) and particular care has been taken on the design aspects of this device. Currently, there are only two hard X-ray beamlines in operation at ELETTRA, which share the same wiggler exit port, with an energy range of 4–22 keV. The new exit port will be fed by a superconducting wiggler and the energy range of XRD2 will be slightly higher (8–35 keV) than beamlines working at present, to make it possible complementary experiment sets.

The original idea was to modify the old monochromator project of the X-ray diffraction beamline, but soon it has been realized that the different energy range gave the possibility of a more compact and robust design, which in turn allows a cost reduction and hopefully a simplified operation and maintenance.

2. Basic concept

The working principle of a double crystal monochromator (DCM) is the well-known Bragg reflection from two parallel crystals. The energy of the exit X-ray beam is a function of the Bragg angle θ_B (figure 1a), and the resulting angular

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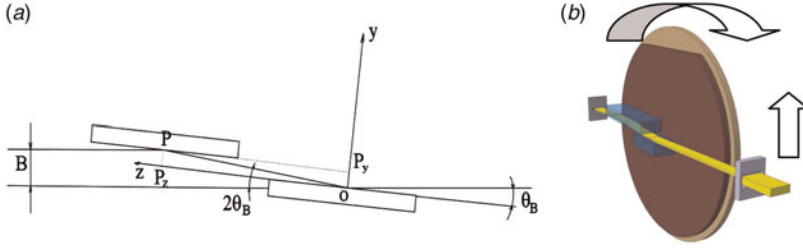


FIGURE 1. (a) Beam path in a DCM. (b) Mask compensation.

range with silicon crystals Si(111) is about $3^\circ < \theta_B < 14.5^\circ$ in the XRD2 case (8–35 keV). With reference to the Oyz axis system of figure 1(a), simple geometrical considerations allow us to derive the position P of the reflected beam on the second crystal with the following equations:

$$y_P = OP_y = \frac{B}{2 \cos(\theta_B)}, \quad (1)$$

$$z_P = OP_z = \frac{B}{2 \sin(\theta_B)}, \quad (2)$$

In particular from equation (1) it can be recognized that y_P is the distance between the two crystals. Therefore, if we keep constant y_P , it follows that $B = B(\theta_B)$.

The DCM is normally designed to have a fixed output beam during the scan. This is usually accomplished by the control of the distance y_P following equation (1). Moreover the second crystal is usually moved in the z -direction with equation (2) in order to limit its dimensions. Since the stated angular range has a limited impact on the offset B , a solution with constant $y_P = K$ was studied. The value of K was carefully minimized (6.5 mm) because of the obvious advantages on both ΔB and Δz_P . In this way, it is possible to use a fixed second crystal of length $L = 150$ mm and with consequent ΔB of about 400 μm in the scan range.

However, the requirement of a fixed exit beam is still desirable and therefore a different solution has been studied as described in figure 1(b). The basic idea is to ‘move’ the entrance beam in the opposite direction (and with the same law) of the function of the offset variation $\Delta B = \Delta B(\theta_B)$.

The vertical movement of the entrance beam is accomplished by a movable mask that cuts the incident beam at different heights during the scan. This apparent movement of the entrance beam is reasonable for small movement of the mask. In our case, the calculated photon flux variation in the centre beam is about 1 %, while on the edges the variation is under 10 %. The difference is due to the fact that the beam is Gaussian in the vertical direction.

3. General aspects of the monochromator

The overall design of the DCM was inspired by the reduction of the active degrees of freedom of the crystals, with the target of a robust design, which in turn can provide a limitation of the system instabilities during the scans, reduction of complexities and cost.

Since the second crystal has no translational movements, the system behaves essentially as a channel cut system, which in principle leads to a very stable system

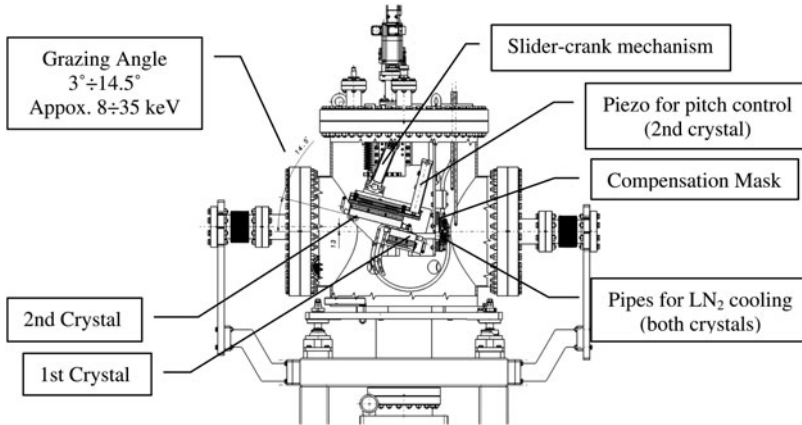


FIGURE 2. XRD2 monochromator cross-section.

(Kupp *et al.* 2003) with limited vibrations and drifts due to secondary movements during the scan. The overall system is described in figure 2. The first crystal is directly clamped to a base plate supported by two lateral slabs containing the bearings for the main rotation axis. This axis is supported in turn by two vertical arms fixed to the top flange (figure 3a).

The second crystal is mounted on a gimbal system described in figure 3(b). The two axes of rotation cross in the middle of reflective surface of the second crystal and are kept in position by means of the short vertical arms of figure 3(b). Flexural pivots are used as bearings and the mechanism allows us to control the roll and pitch of the crystal. The latter is controlled by means of a piezoelectric-motor fixed on the top plate and pushing the bottom plate of the gimbal against a spring element (figure 3b).

Finally, the gimbal assembly is fixed to the lateral slabs to form, together with the first crystal base plate, a cradle rotating around the main horizontal axis.

The movement is actuated by a linear feed-through that drives a slider-crank mechanism that can be seen in figure 2.

Both crystals are cryogenically cooled by means of two independent LN₂ circuits. Copper pipes with square section are kept in contact with the silicon bodies with the interposition of Indium foils (indirect cooling). The cryogenic-cooling system

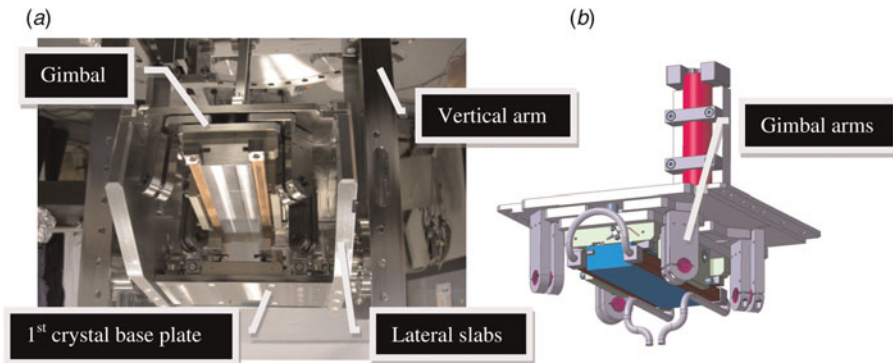


FIGURE 3. (a) XRD2 monochromator during assembly. (b) Second crystal gimbal system.

was chosen because of the relatively high power absorption of the first crystal (about 400 W). In this way, it is possible to keep the silicon crystals' temperatures under about 130 K, a temperature range in which the ratio α/k for silicon (α = coefficient of thermal expansion, k = thermal conductivity) is very low (Marion *et al.* 2006) and the thermal distortions can be minimized.

The front mask is water cooled with a single copper pipe circuit directly brazed on a copper body.

The last degree of freedom to be controlled is the vertical movement of the mask. Although it would be possible to add a motor to move the mask with a feedback control from the encoder, a self-compensation scheme was studied and it will be described in the next section.

4. Self-compensation mechanism

The idea of a self-compensation mechanism came out when studying the law of movement of the slider-crank mechanism as in the sketch of figure 4(a).

In the sketch, B_2 is the small end of the connecting rod B_1B_2 , while O is the centre of rotation lying on the surface of the first crystal. Once the linear dimensions are known, it is possible to derive the law $y'_{B_2} = f(\theta_B)$ that we omit herein for simplicity, but we want to focus on the movement of the bar P_1P_2 . The bar is free to rotate in P_1 , positioned at a distance D downward to the centre of rotation O . The bar is kept horizontal by the sleeve in S_1 and the sleeve itself is rigidly connected to a plate that is constituted by the movable part of a vertical stage (mask support). The practical mechanical solution is visible in figure 4(b).

If the distance D between P_1 and O is double the distance between the two crystal reflective planes (i.e. $2 y_P$), it is easy to recognize that

$$y'_{\text{mask}} = D - D \cos(\theta_B) = 2y_P(1 - \cos(\theta_B)). \quad (3)$$

If we remember expression (1), the beam offset can be expressed as

$$B = 2y_P \cos(\theta_B), \quad (4)$$

which gives the decreasing trend of the offset B as the grazing angle θ_B increases.

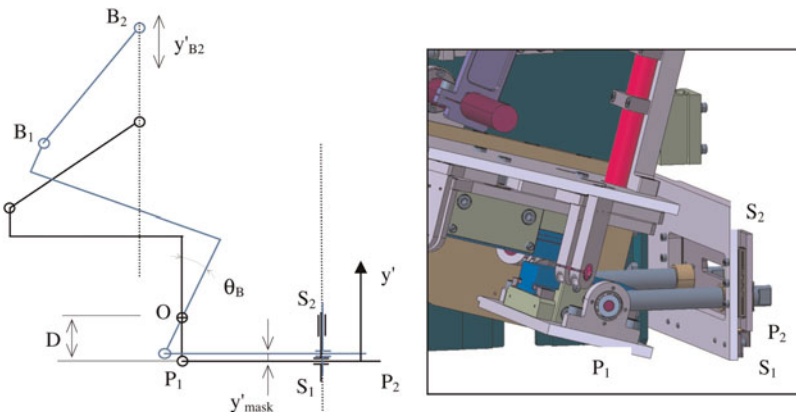


FIGURE 4. (a) Compensation scheme. (b) Practical mechanical solution.

Since B is the difference between the beam height, we have

$$y'_{\text{out}} - y'_{\text{in}} = 2y_P \cos(\theta_B). \quad (5)$$

Usually y'_{in} is the constant ($y'_{\text{in}} = C$) and therefore $y'_{\text{out}} = f(\theta_B)$. By 'moving' the incoming beam with a law

$$y'_{\text{in}} = C + y'_{\text{mask}} = C + 2y_P(1 - \cos(\theta_B)). \quad (6)$$

By substituting equation (6) into (5), we obtain:

$$y'_{\text{out}} = C + 2y_P = \text{constant} \quad (7)$$

and the self-compensation is obtained.

It is worth noting that the described mechanism has somehow a general validity, in the sense that it can be used, in principle, slightly modified, to achieve the compensation by moving the distance y_P between crystals, of course maintaining the mask fixed.

5. Conclusions

The mechanical system of the XRD2 monochromator is in the final assembly phase, when these notes are written; therefore, only limited conclusions can be taken on system performances. However, the overall cost of the mechanical system has been significantly reduced for several reasons, the compactness of the system, the simplification of the main rotary actuation that avoids the traditional goniometer with the needed differential pumping system, the reduced degree of freedom and the relative limited number of pieces.

Although it is not possible to draw conclusions on system precision, the pre-checks during the assembly phase have shown the consistency of the system with the design parameters and no particular problem arose with the functionality of the active degree of freedom that let us be confident for the next test phase.

Acknowledgements

Many thanks to the CINEL[®] staff for the useful suggestions and implementations during the construction phase of the monochromator prototype.

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